8.0 Solving Time dependent problems

8.1 First order differential eqs: "Cahn-Hilliard equation"

- Goal: model "spinodal decomposition" of a solid solution of A & B

Let: \( p_A, p_B \) denote concentrations of A, B

Let \( c = \frac{p_A - p_B}{p_A + p_B} \) \(-1 < c < 1\)

\(c = 1 \Rightarrow \) pure A
\(c = -1 \Rightarrow \) pure B

Let free energy be \( G(c) = \frac{1}{4} (c^2 - 1)^2 + K \sqrt{\frac{dc}{dx} \cdot \frac{dc}{dx}}\)

Bulk \hspace{2cm} Interface energy
Free energy has minima if $c = \pm 1$

Evolution equations for $c$

$$\frac{dc}{dt} = \frac{\delta D}{\delta x_i} \frac{\delta \mu}{\delta x_i} + f(c)$$

$$\mu = \frac{SG}{S} = c(c^2 - 1) - \kappa \frac{d^2 c}{dx_i dx_i}$$

"Chemical Potential"

$E = 0 \ c = 0 \rightarrow$ Phase separation $\rightarrow$ Coarsening
- Initial conditions \( c(t=0, x) = A \sin kx, \sin kx \)  

- Boundary conditions (symmetry) \( \frac{\partial c}{\partial x_i} \bigg|_{x_i=0} = 0 \)  
on all 4 boundaries

**Goal:** Solve for \( \mu(t), c(t) \)

**Weak Form:** Let \( \delta \mu, \delta c \) be two differentiable test functions

\[
\int \left\{ \mu - f(c) + k \frac{\partial^2 c}{\partial x_i \partial x_i} \right\} \delta \mu \, dv = \int \left\{ \left( \mu - f(c) \right) \delta \mu - k \frac{\partial c}{\partial x_i} \frac{\partial \delta \mu}{\partial x_i} \right\} dv \\
\int \left\{ \frac{\partial c}{\partial t} \frac{\partial}{\partial x_i} \delta c \right\} \delta c \, dv = \int \left\{ \frac{\partial c}{\partial t} \frac{\partial c}{\partial x_i} + \frac{\partial^2 c}{\partial t \partial x_i} \frac{\partial \delta c}{\partial x_i} \right\} dv = 0
\]

\[ \forall \delta c, \delta \mu \]


Introduce FE interpolations

\[ \mu = N^a \mu^a \quad S\mu = N^a S\mu^a \]
\[ c = N^a c^a \quad S\xi = N^a S\xi^a \]
\[ N^a \]

Discrete system

\[ M_{ab} \mu^b(t) - F^a (c^b) - K_{ab} c^b(t) = 0 \quad (1) \]

\[ M_{ab} \frac{dc^b(t)}{dt} - D K_{ab} \mu^b(t) = 0 \quad (2) \]

\[ M_{ab} = \int_{R} N^a N^b dV \]
\[ K_{ab} = \int_{R} \frac{\partial N^a}{\partial x_i} \frac{\partial N^b}{\partial x_i} dV \]

\[ F^a = \int_{R} N^a f(c) dV \quad c = \xi N^a c^a \]
Time Integration

FEA nearly always uses simple Euler scheme
- Estimate time derivatives; multiply by $\Delta t$

Assume $\mu^a, c^a$ known at time $t$
Calculate $\Delta \mu^a, \Delta c^a$ during $\Delta t$
Update, repeat.

We need to find $\frac{dc^a}{dt}$: Could use

1. Use $\mu^a$ at time $t$ ("Explicit")
2. """" """" $b + \Delta t$ ("Implicit")
3. Combination

We can set up a general scheme
(2) in discrete form

\[ M_{ab} \frac{\Delta c^b}{\Delta t} - D K_{ab} \left\{ (1-\theta) \mu^b + \theta (\mu^b + \Delta \mu^b) \right\} \]

\[ 0 < \theta < 1 \]

\[ \theta = 0 \Rightarrow \text{Explicit} \]

\[ \theta = 1 \Rightarrow \text{Implicit} \]

\[ \theta = \frac{1}{2} \Rightarrow \text{midpoint} \]

(1) \[ M_{ab} (\mu^b + \Delta \mu^b) - F^a (c^b + \Delta c^b) - K K_{ab} (c^b + \Delta c^b) = 0 \]
Implementatin

Goal: re-write in a form best suited for use

Note that our global equation system has same general structure as for mechanics

\[ \mathbf{R}_i \mathbf{A} \mathbf{U} + \mathbf{A} \mathbf{U} \Delta \mathbf{U} = 0 \]

\( \mathbf{U} \) - vector of unknowns \([ \mu^1, \ldots, \mu^3, c^1, \ldots, c^3 ]\)

\( \Delta \mathbf{U} \) - vector of increments

\( \mathbf{R}_i \) is \( i \)th equation for \( a \)th node

Rearrange in usual form
Note equations contain \( \mu, c, \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} \).

Hence define \( f = [\mu, c, \frac{\partial u}{\partial x_i}, \frac{\partial u}{\partial x_j}] \).

Define \([B]\) such that \( f = [B] U e^t \).

Now note that our equation system can be expressed as

\[ 5 f^T q = 0 \]

where \( q \) is (Get from weak form)
\[ q = \begin{bmatrix}
\mu + \Delta \mu - f(x) \\
\Delta c \\
\frac{\Delta c}{\Delta t} \\
-k \frac{\partial (c + \Delta c)}{\partial x_1} \\
-k \frac{\partial (c + \Delta c)}{\partial x_2} \\

\nabla \frac{\partial (\mu + \Theta \Delta \mu)}{\partial x_1} \\
\nabla \frac{\partial (\mu + \Theta \Delta \mu)}{\partial x_2}
\end{bmatrix}
\]

Recall also
\[ s_f = [B] S_u \]

\[ R^e l = \int_{\Omega} [B]^T q \, dV \]

Hence
This is identical to stress analysis with $q$ replacing $g$.

Nonlinear system $RU = 0$

Solve with Newton-Raphson

Guess $U = W$

Correct $[K]dW = -[R][W]$ [B]

Where $[K] = \frac{\partial \mathbf{R}}{\partial \mathbf{U}} = \int C[B]^T \frac{\partial \mathbf{q}}{\partial \mathbf{U}} \frac{\partial \mathbf{p}}{\partial \mathbf{U}} dV$ [D]
Here \( [D] = \begin{bmatrix} \frac{\partial q_1}{\partial p_1} & \frac{\partial q_1}{\partial p_2} & \frac{\partial q_1}{\partial p_3} \\ \frac{\partial q_2}{\partial p_1} & \frac{\partial q_2}{\partial p_2} & \frac{\partial q_2}{\partial p_3} \\ \frac{\partial q_3}{\partial p_1} & \frac{\partial q_3}{\partial p_2} & \frac{\partial q_3}{\partial p_3} \end{bmatrix} \)

\[
[D] = \begin{bmatrix}
1 & -\frac{df}{dc} & 0 & 0 & 0 & 0 \\
0 & 1/\Delta t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\kappa & 0 \\
0 & 0 & 0 & 0 & 0 & -\kappa \\
0 & 0 & 0 & 0 & \theta D & 0 \\
0 & 0 & 0 & 0 & \theta D & 0 \\
\end{bmatrix}
\]

\[df / dc = 3(c + \Delta c)^2 - 1\]

**Summary:** UEL computes \( - \int_{\text{rel}} \{B\}^T \{\eta\} = -\{R\} \quad (K) = \int_{\text{rel}} \{C\}^T [D] \{B\} \, dV \)